LA-UR -85-4172

CONF-860204--24

LA-UR--85-4172

DE86 004722

TITLE: HYDROGEN-COMBUSTION ANALYSES OF LARGE-SCALE TESTS

AUTHOR(S): R. G. Gido
A. Koestel

SUBMITTED TO: Thermal Reactor Safety Meeting,
February 2-6, 1986
San Diego, CA

HYDROGEN-COMBUSTION ANALYSES OF LARGE-SCALE TESTS

R. G. Gido and A. Koestel

Los Alamos National Laboratory
University of California

SUMMARY This report uses results of the large-scale tests with turbulence performed by the Electric Power Research Institute at the Nevada Test Site to evaluate hydrogen burn-analysis procedures based on lumped-parameter codes like COMPARE-H2 and associated burn-parameter models. The test results (a) confirmed, in a general way, the procedures for application to pulsed burning, (b) increased significantly our understanding of the burn phenomenon by demonstrating that continuous burning can occur and (c) indicated that steam can terminate continuous burning. Future actions recommended include (a) modification of the code to perform continuous-burn analyses, which is demonstrated, (b) analyses to determine the type of burning (pulsed or continuous) that will exist in nuclear containments and the stable location if the burning is continuous, and (c) changes to the models for estimating burn parameters.

I. INTRODUCTION

With respect to hydrogen-burn-analysis procedures, this report evaluates the applicability of the NTS test results, the capability of the COMPARE-H2 code, and current procedures for specifying burn parameters. This work was performed under the auspices of the US Nuclear Regulatory Commission and is reported more completely in Ref. 1. The evaluation is accomplished by performing code analyses of the recently-completed Electric Power Research Institute (EPRI) tests at the Nevada Test Site (NTS),[2] which were conducted in a large volume (73 600 ft^3) to represent the large geometric scale of nuclear containments.

In general, the hydrogen-burn analysis procedures used involve application of codes and burn-parameter models. For our analyses, we use COMPARE-H2,[3] the hydrogen-burn version of the COMPARE code,[4] and our previously-developed hydrogen-burn models[5] for the estimation of burn parameters.

Basic assumptions used in COMPARE-H2 [and similar codes like CLASIX (Ref. 6) and HECTR (Ref. 7)] are that the nodes are homogeneous and in thermodynamic equilibrium and that the flow between nodes can be estimated with relatively simple flow models. In our hydrogen-burn models, the combustion occurs in an atmosphere in which turbulence dominates the physical phenomena important to burning. Note that the available evidence indicates that mixing processes are adequate to allow simulation with a code such as COMPARE-H2 if containment engineered-safety systems such as fans and sprays are operating.

II. HYDROGEN BURN PARAMETERS

The three basic burn parameters used by codes like COMPARE-H2 when performing hydrogen-burn analyses are burn time, flammability limit, and fraction burned.

II.A Burn Time

By definition, (a) burn velocity or deflagration rate will be relative to the unburned mixture, (b) flame speed will be relative to the walls, and (c) burn time will be the flame propagation distance divided by the flame speed. Reference 5 discusses two turbulent-burning flame speeds that can be used to compute the burn time for pressure-pulse burning analysis: the turbulent burn velocity with respect to the unburned mixture, S_T, and the flame speed with respect to the vessel wall FS, which is S_T increased to account for gas expansion.

Table XI.5-I presents the test conditions, test results and an analysis that compares the flame speed indicated by the test with S_T and FS. The comparison of the predicted and measured flame speed indicates that the actual flame speed for these tests is bracketed by S_T and FS. However, it is not clear which should be used for compartments in general because (a) geometries and flow conditions are varied and complex, and (b) NTS results are test specific with application restricted probably to geometries and flow conditions similar to those for NTS. Note that the flame speed increased to account for the gas expansion (FS) should result in maximum pressure peaks for pulse burning because the time of burning is less, which results in less energy transfer to heat sinks and less pressure-relief flow out of the compartment. The burn-time parameter has limited significance for continuous burning.

II.B Flammability Limit & Mean Concentration at Ignition

We define the flammability limit as the local H_2 concentration at the igniter when ignition is initiated, which is different from the volumetric mean concentration at ignition (X_o). X_o is related to the flammability limit and the concentration gradient, which depends on turbulence and scale as discussed in Ref. 5. For example, (a) with good mixing, X_o is higher than the flammability limit, and (b) with poor mixing, X_o could be lower than the flammability limit because burning could occur at a high local concentration of hydrogen.

The NTS test results indicate a value of ~5% for the flammability limit based on the fraction of hydrogen burned (for premixed tests with turbulence) vs the hydrogen concentration as shown in Fig. XI.5-1. This plot shows that a fraction-burned value of zero corresponds to a hydrogen concentration of ~5%, thereby defining the flammability limit. This observation is confirmed by NTS test results for the the ratio of maximum to initial pressures vs hydrogen concentration going to a minimum level of combustion (pressure ratio of one) at a hydrogen concentration of ~5%, see Ref. 1.

It appears that a reasonable estimate of the mean concentration at ignition (X_o) can be obtained from (a) the turbulent-mixture flammability limit of 4 to 5% depending on the steam concentration and (b) Ref. 5 to account for the effects of turbulence and scale (compartment size) on concentration gradient.

II.C Fraction Burned

Figure XI.5-1 shows the fraction burned (F) indicated by the NTS tests with turbulence and compares these results with our curve, developed in Ref. 5. Note that the main difference between the curves is the flammability limit (where F goes to zero), which is caused probably by the high steam concentrations of the NTS tests. The curve comparison of Fig. XI.5-1 indicates that (a) the fraction-burned curves should be made to depend on the steam concentration, and (b) the NTS fraction-burned dependence on X_o (i.e., the curve shape) is similar to that based on the model developed in Ref. 5, which is interpreted as verification of the basic model premise that burning is restricted by heat loss (thermal radiation).

III. COMPARISON WITH NTS RESULTS

This section compares NTS-measured and COMPARE-H2-calculated results only for tests with turbulence created by fans, sprays, or injected-flow velocity. Tests with turbulence are emphasized because the most appropriate application of the code is to analyze containment atmospheres with significant turbulence created by sprays and recirculating fans.

III.A Premixed

COMPARE-H2 calculated results are presented for NTS premixed tests P-2 and P-3 for the initial conditions of Table XI.5-I. These tests were used for comparison because they had (a) turbulence generated by fans and sprays, and (b) central ignition, which provides a simple geometry for flame propagation. Also compared are the calculated and measured pressure and temperature maxima and the pressure at 100 s. The latter is done to evaluate the code ability to account for the decrease in pressure with time. Burn parameters used were based on information given in Ref. 2, which is the basic NTS reference, and Ref. 8, which suggests different NTS burn times and burn fractions. The burn-parameter models used are presented in Ref. 5.

III.A.1 Test P-3 (Fans)

Table XI.5-II presents calculated results for several combinations of the fraction burned, burn time and models used to calculate the heat transfer to heat sinks. Figure XI.5-2 shows the measured and calculated pressure variations.

III.A.2 Test P-2 (Sprays)

Table XI.5-III presents calculated results for several combinations of the fraction burned, burn time, and models used to calculate the heat transfer to heat sinks. Figure XI.5-3 shows the measured and calculated pressure variations. Note that using the Ref. 2 burn fraction and burn time results in calculated maximum pressure and temperature significantly below that measured. Possible explanations for the differences are that the burn fraction was measured erroneously, as indicated in Ref. 8, and that the mixed mean concentration at ignition (X_o), is wrong, which has a large effect on pressure and temperature increase. Table XI.5-IV is presented also as a sensitivity study of the effect of energy removal models.

III.B Continuous Injection (Test C-S1)

COMPARE-H2 calculated and measured pressures are compared for continuous injection test C-S1 because the turbulence generated by the injected fluids appears to be high enough to have created a well-mixed atmosphere, a condition appropriate for application of the code. Continuous- and pulsed-burn calculations were performed.

III.B.1 Continuous vs Pulsed Burning

The COMPARE-H2 continuous burning calculation shown in Fig. XI.5-4 is based on burn initiation at 285 s as measured,[2] burn termination at 900 s as indicated by the measured pressure profile, initial conditions (zero time) as measured,[2] an arbitrary burn rate of 0.02 moles-H_2/sec, and the Los Alamos heat-transfer model; see Ref. 1.

The COMPARE-H2 pulsed-burning calculation (compared with the measured pressures) shown in Fig. XI.5-5 is based on turbulence assumed to be similar to that estimated to be generated by the fans, burn initiation at a mean hydrogen concentration of 0.050%, burn fraction of 0.50 based on the burn model presented in Ref. 5, burn time of 8 s (based on central ignition and a flame speed from the turbulent burn velocity increased to account for expansion of the burned gases; see Table XI.5-I), the same initial conditions as for the continuous-burn calculation, and terminating the pulsed-burn calculation at ~41% steam.

Comparison of the relative values reveals:

- A maximum measured pressure of 28 psia in comparison to 31.0 and 35.4 for the continuous and pulsed calculations, respectively.
- A maximum measured temperature of 385°F in comparison to 408 and 776 for the continuous and pulsed calculations, respectively.
- The fraction of the total hydrogen available that is burned is 0.39 and 0.31 for the pulsed and continuous burn calculations, respectively.
- Higher pressure and temperature peaks for the pulsed-burn calculation because burn rates are between 0.6 and 0.7 moles-H_2/s in comparison to the continuous rate of 0.02.
- Note that the continuous-burn integrated-mean pressures and temperatures would have transient profiles similar to those for the continuous-burn calculations.

IV. CONCLUSIONS AND RECOMMENDATIONS

The conclusions and recommendations presented below are discussed under separate sections that deal with the NTS tests, the COMPARE-H2 code, and the models needed to estimate burn-parameter specifications for the code. Atmospheres with significant turbulence were emphasized because this is the condition most appropriate for application and assessment of the COMPARE-H2 code.

Our conclusions and recommendations regarding the NTS hydrogen-burn tests follow:

- The test results have confirmed, in a general way, the hydrogen-burn analysis procedures that we have been using.
- The tests have increased significantly our understanding of the burn phenomenon by providing information showing that continuous burning can occur and steam can terminate continuous burning.
- Test results should be investigated to establish the reason for burn termination of the continuous-burn tests. In particular, it should be established whether the cause of burn termination was the increased steam level, which is suggested by our analyses.

Our conclusions and recommendations regarding the COMPARE-H2 code are:

- Pulsed-burning maxima for an enclosed vessel are predicted well if the burn-parameter specifications are known, see below.
- Heat-transfer models are adequate for estimating pressure and temperature maxima if adequate information is provided to specify the heat sinks.

- COMPARE-H2 should be modified to perform continuous-burning analyses because this type of burning might occur in an nuclear containment and the resulting effect (for example, on equipment qualification) might require evaluation.

Our conclusions and recommendations regarding the models needed to estimate burn-parameter specifications for the COMPARE-H2 code are:

- Analyses should be performed to determine if pulsed, continuous, or both types of burning will occur in nuclear containments.
- For continuous burning, analyses should be performed to determine the possible location(s) of the stable continuous burn in nuclear containments.
- Basic concepts developed before the NTS tests (see Ref. 5) were verified.
- Flammability limit values >5% should be used with an accounting made for the effect of steam.
- For the prediction of pressure and temperature peaks for pulsed-burning analyses of unvented volumes, the higher fraction-burned curve presented in Fig. XI.5-1 should be considered for use because the burning of more hydrogen and, therefore, higher pressures and temperatures would result. Note that most of the NTS data was correlated by the lower fraction-burned curve in Fig. XI.5-1.
- For the prediction of maximum pressure and temperature peaks for pulsed-burning analyses of unvented volumes, the burn time should be estimated from the maximum flame speed model presented in Ref. 5 because this would result in a shorter burn time, less energy removal, and, therefore, higher pressures and temperatures.

REFERENCES

1. Attachment titled "COMPARE Hydrogen-Burn-Analysis Code Evaluation" to letter Q-9-85-L-308 to Charles G. Tinkler, US Nuclear Regulatory Commission, from Richard G. Gido, Los Alamos (May 8, 1985).
2. "Large-Scale Hydrogen Combustion Experiments," Draft of Final Report for Research Project 1932-11, Electric Power Research Institute.
3. Attachment titled "Input Description for the Hydrogen-Burn Version of COMPARE" to letter Q-7-84-214 to Charles G. Tinkler, US Nuclear Regulatory Commission, from Richard G. Gido, Los Alamos (May 2, 1984).
4. R. G. Gido, G. J. E. Willcutt, Jr., J. L. Lunsford, and J. S. Gilbert, "COMPARE-MOD 1 Code Addendum," Los Alamos Scientific Laboratory report LA-7199-MS (NUREG/CR-1185), Addendum 1 (August 1979).
5. R. G. Gido and A. Koestel, "Parameters for Containment Hydrogen-Burn Analysis," Joint ANS/ASME Conference on Design Construction and Operation of Nuclear Power Plants, Portland, OR (August 5-8, 1984).
6. "The CLASIX Computer Program for the Analysis of Reactor Plant Containment Response to Hydrogen Release and Deflagration," Offshore Power Systems Report No. OPS-36A31 (October 1981).
7. A. L. Camp, M. J. Wester, and S. E. Dingman, "HECTR Version 1.0 User's Manual," Sandia National Laboratories report NUREG/CR-3913, SAND84-1522 (February 1985).
8. A. C. Ratzel, "Data Analyses for Nevada Test Site (NTS) Premixed Combustion Tests," Sandia National Laboratories report NUREG/CR-4138, SAND85-0135 (May 1985).

TABLE XI.5-I

FLAME-SPEED ANALYSIS OF NTS TESTS P-2 AND P-3

	NTS Test P-2	NTS Test P-3
Conditions		
H_2/H_2O v/o at ignition	5.8/14.3	5.8/14.4
Initial press., psia	13.2	14.2
Initial temp. T_o, °F	124.	117.
Igniter location	Center	Center
Sprays(S)/Fans(F)	S	F
Results		
Pressure rise, psi	15.3	11.3
Max. temp. measured, °F	880.	600.
Adiabatic temp. (T_{ad}), °F	1216.	1218.
Fraction burned(F)	0.43	0.44
Press. rise time(t_b) Ref. 2/Ref. 8, s	5./4.1	13./12.3
Analysis[a]		
Turbulence(u′),[b] ft/s	2.07	1.43
Turbulent burn velocity(S_T),[c] ft/s	3.45	1.88
S_T multiplier(T_b/T_o),[d]	3.45	1.88
Max. flame speed(FS),[e] ft/s	6.22	3.42
Meas. flame speed($u_m = L^f/t_b$) Ref. 2/Ref. 8, ft/s	5.2/6.3	2.0/2.1
Predictions vs measurements		
Ref. 2/Ref. 8: $(S_T - u_m)/u_m$, %	-34./-45.	-6./-10.
Ref. 2/Ref. 8: $(FS - u_m)/u_m$, %	20./-1.	71./63.

Notes–
[a] Reference 5 explains the procedures for determining burn velocity, flame speed and burn time.
[b] Turbulence based on the parameters: Spray - 15.2 gpm, nozzle press. diff. = 40 psi, fall height = 60 ft; Fans - 5000 afm, 16 in. diameter.
[c] $S_T = 1.09 \cdot u' + S_L$, where the laminar burn velocity $S_L = 0.32$ ft/s.
[d] $T_b/T_o = F \cdot (T_{ad}/T_o - 1) + 1$, where T_b = temp. of the burned products, T_o = initial temp., F = fraction burned and T_{ad} = adiabatic temp.
[e] $FS = S_T \cdot T_b/T_o$.
[f] For center ignition used 1/2 = diameter of 32 ft.

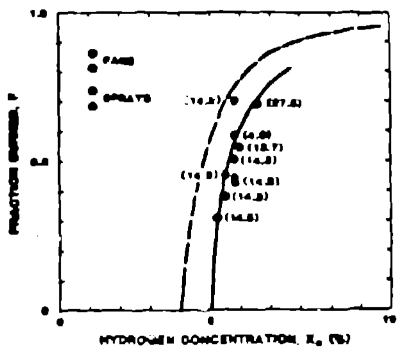

Fig. XI.5-1.
Fraction (F) of hydrogen at ignition consumed during burning vs the volumetric-mean hydrogen concentration at ignition (X_o). Tests are premixed with turbulence generated by sprays (S) or fans (F). Values in parentheses are steam concentration in vol%. Extrapolated to F = 0 indicates a flammability limit of ~5% for the NTS tests. For comparison, the dashed curve shows the F vs X_o based on a mechanistic model and confirmed with small and intermediate test data.[1] The model accounts for the effect of temperature on chemical kinetics (Arrhenius equation), which explains the strong dependence of F on X_o.

TABLE XI.5-II
NTS P-3 (Fans). CALCULATED VS MEASURED RESULTS

Initial Conditions: 5.8 vol% H_2, P_o = 14.0 psia, T_o = 126 °F
Measured Values: P_{max} = 25.1 psia, T_{max} = 690 °F, P_{100} (P at 100 s) = 19.3 psia

Purpose	Calc. No.	F-Burn Frac.	BT-Burn Time, s	HT[a] Model	Max. P, psia	Max. Temp., °F	Calc./Meas. P_{max}	Calc./Meas. T_{max}	Calc./Meas. P_{100}[b]
EPRI[1] F & BT, MRC HT	P3-1	0.44	13.0	MRC	25.8	635	1.03	0.91	1.05
Ref. 8 F & BT, MRC HT	P3-2	0.50	12.3	MRC	27.3	705	1.09	1.02	1.07
Ref. 8 F & BT based on Table 1 max FS,[c] MRC HT	P3-3	0.50	7.6	MRC	27.5	712	1.10	1.04	1.06
Ref. 8 F & BT based on Table 1 S_T^c, MRC HT	P3-4	0.50	13.8	MRC	27.2	702	1.08	1.02	1.08
Ref. 5 F & BT,[d] MRC HT	P3-5	0.74	7.6	MRC	33.2	968	1.32	1.49	1.10
Ref. 8 F & BT, LASL HT	P3-6	0.50	12.3	LASL	25.9	674	1.03	0.97	0.97
Max F, Min BT, MRC HT[e]	P3-7	0.74	7.6	MRC	33.2	968	1.32	1.49	1.10

a MRC HT uses T_{sat} to determine energy removal and h_{fg} to determine the associated condensed mass removed. LASL HT uses T_{bulk} and a mechanistic condensed mass removal model that results in less mass/energy removal. See Ref. 1.
b Pressure at 100 s used to characterize shape of the pressure curve.
c Table 1 presents mechanistic predictions for turbulent burn velocity (S_T) and maximum flame speed (FS) that provide burn time by dividing these values into the assumed propagation distance (for central ignition) of 26 ft.
d Reference 5 F corresponds to the higher F curve of Fig. 1 and the Ref. 5 BT corresponds to the max flame speed (FS) of Table 1.
e Parameters recommended to obtain maximum peak pressure and temperature.

TABLE XI.5-III
NTS P-2 (Sprays): CALCULATED VS MEASURED RESULTS

Initial Conditions: 5.8 vol% H_2, P_o = 12.8 psia, T_o = 123 °F
Measured Values: P_{max} = 28.5 psia, T_{max} = 880 °F, P_{100} (P at 100 s) = 15.0 psia

Purpose	Calc. No.	F-Burn Frac.	BT-Burn Time, s	HT[a] Model	Max. P, psia	Max. Temp., °F	- -Calc./Meas.- - P_{max}	$T_{max}-T_o$	P_{100}^b
EPRI[2] F & BT, NRC HT	P2-1	0.43	5.0	NRC	21.6	513	0.76	0.51	0.94
Ref. 8 F & BT, NRC HT	P2-2	0.70	4.1	NRC	27.8	798	0.98	0.89	0.99
Ref. 8 F & BT based on Table I max FS,[c] NRC HT	P2-3	0.70	4.2	NRC	27.9	801	0.98	0.90	0.99
Ref. 8 F & BT based on Table I S_T^c, NRC HT	P2-4	0.70	7.5	NRC	26.3	705	0.92	0.76	0.99
Ref. 5 F & BT,[d] NRC HT	P2-5	0.74	4.2	NRC	29.6	886	1.04	1.01	1.00
Ref. 8 F & BT, LASL HT	P2-6	0.70	4.1	LASL	26.9	765	0.94	0.85	0.91
Max F, Min BT, NRC HT[e]	P2-7	0.74	4.2	NRC	29.6	886	1.04	1.01	1.00

a NRC HT uses T_{sat} to determine energy removal and h_{fg} to determine the associated condensed mass removed. LASL HT uses T_{bulk} and a mechanistic condensed mass removal model that results in less mass/energy removal. See Ref. 1.
b Pressure at 100 s used to characterize shape of the pressure curve.
c Table I presents mechanistic predictions for turbulent burn velocity (S_T) and maximum flame speed (FS) that provide burn time by dividing these values into the assumed propagation distance (for central ignition) of 26 ft.
d Reference 5 F corresponds to the higher F curve of Fig. 1 and the Ref. 5 BT corresponds to the max flame speed (FS) of Table I.
e Parameters recommended to obtain maximum peak pressure and temperature.

TABLE XI.5-IV
NTS P-2 (Sprays): EFFECT OF HEAT SINKS

Initial Conditions: 5.8 vol% H_2, P_o = 12.8 psia, T_o = 123 °F
Reference Calc. (Calc P2-7 from Table III) has: Frac. Burned = 0.70, Burn Time = 4.2 s, NRC HT

Variation	Calc. No.	Max. P, psia	Max. Temp., °F	P_{100}, psia	- Sensitivity(%)[a] - P_{max}	$T_{max}-T_o$	P_{100}^b
None - Reference Calc. (P2-2 from Table III)	P2-2	27.8	798	14.9	---	---	---
Time step × 0.5	P2-11	27.8	795	14.8	0.0	-0.4	-0.7
Spray drop size × 2	P2-12	29.0	876	15.3	4.3	11.5	2.6
Spray flow rate × 0.5	P2-13	28.7	853	15.6	3.2	8.1	4.7
No spray	P2-14	29.6	916	19.2	6.5	17.5	28.8
No radiation	P2-15	28.1	811	15.0	1.1	1.9	0.7
0.5 × heat transfer h×A	P2-16	27.9	795	15.5	0.4	-0.4	4.0

a Sensitivity is 100 × (Calc. value - Ref. Calc. value)/(Ref. Calc. value).
b Pressure at 100 s used to characterize shape of the pressure curve.

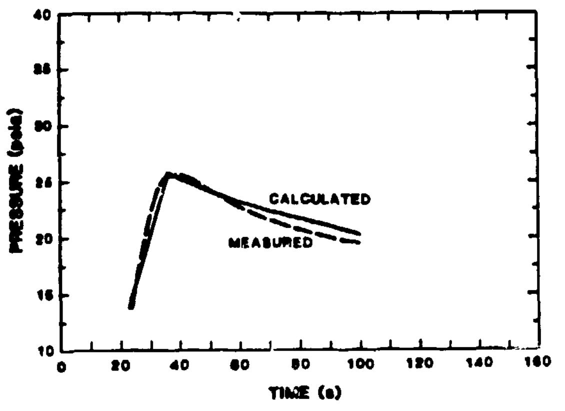

Fig. XI.5-2.
NTS premixed test P-3 (Calc. No. P3-1) COMPARE-H2 calculated pressure vs time using burn initiation at 0.058 %, a burn fraction of 0.44, a burn time of 13.0 s and the NRC heat transfer models, see Ref. 1. The dashed line is the measured pressure variation.

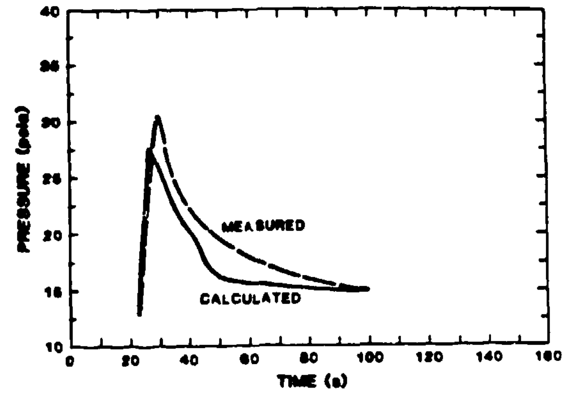

Fig. XI.5-3.
NTS premixed Test P-2 (Calc. No. P2-2) COMPARE-H2 calculated pressure vs time using burn initiation at 0.058 %, a burn fraction of 0.70, a burn time of 4.1 s and the NRC heat-transfer models, see Ref. 1. The dashed line is the measured pressure variation.

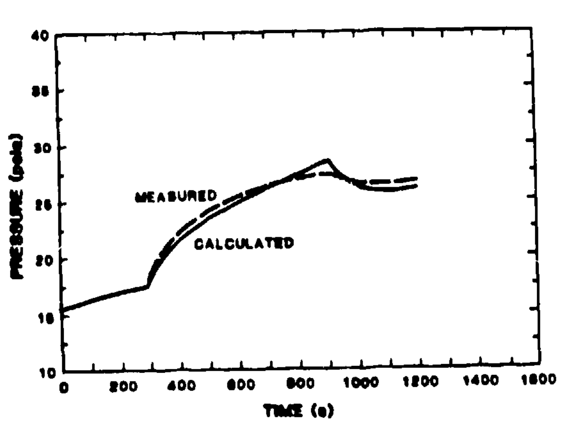

Fig. XI.5-4.
NTS continuous injection Test C-S1 COMPARE-H2 calculated pressure vs time with continuous burning at 0.02 moles-H_2/s starting at 285 s and ending at 900 s. The LASL heat-transfer models were used, see Ref. 1. The dashed curve is the measured pressure variation. Note that the calculated maximum (900 s) pressure (psia) is 28.5 in comparison to the measured value of 28.0.

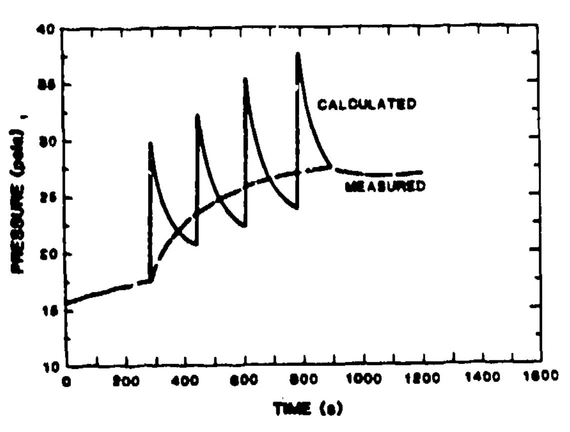

Fig. XI.5-5.
NTS continuous injection Test C-S1 COMPARE-H2 calculated pressure vs time for pulsed burning with (a) initiation at a mean hydrogen concentration of 0.050 %, (b) fraction burned of 0.50, (c) burn time of 8 s and (d) heat transfer to sinks based on the Los Alamos heat-transfer models, see Ref. 1, and (d) termination of the burn at a steam concentration of ~41 . The dashed curve is the measured pressure variation for the test, which experienced a continuous burn that terminated at 900 s and resulted in a maximum pressure of 28 psia.